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ELECTRONIC STRUCTURE OF SILICON NANOCRYSTALS AS A FUNCTION OF PARTICLE SIZE*

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X-ray absorption (XAS) and photoemission spectra (PES) have been measured with synchrotron radiation on thin films of Si nanoclusters with an average size ranging from from 1 to 10's of nanometers. The Si nanocrystals have been synthesized in situ by thermal vaporization of Si in an Ar buffer gas, followed by subsequent exposure to atomic hydrogen to passivate the surface. High resolution transmission electron microscopy revealed that these nanoclusters are crystalline and approximately spherical in shape. Characterization of the size and morphology of the synthesized material was done in situ using STM and ex-situ using atomic force microscopy. We find the size distribution (FWHM) of the particles is approximately 30% of the average size. A comparison of the XAS for Si nanocrystals with crystalline Si shows that the L-edge in the nanocrystals is blue-shifted and broadened relative to the L-edge in bulk Si, consistent with a distribution of quantum confinement energies in the conduction band of the nanocrystalline Si. The blue shift of the silicon L-edge absorption varied from 0.10 eV for clusters that were 3.5 nm in diameter to 0.38 eV for clusters that were 1.5 nm in diameter. PES measurements are in progress to determine the effect of decreasing particle size on the valence band maximum of the silicon clusters. We compare these experimental results to recent theories predicting quantum confinement effects in the bandgap of silicon nanostructures.

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